

FIG. 1(a)

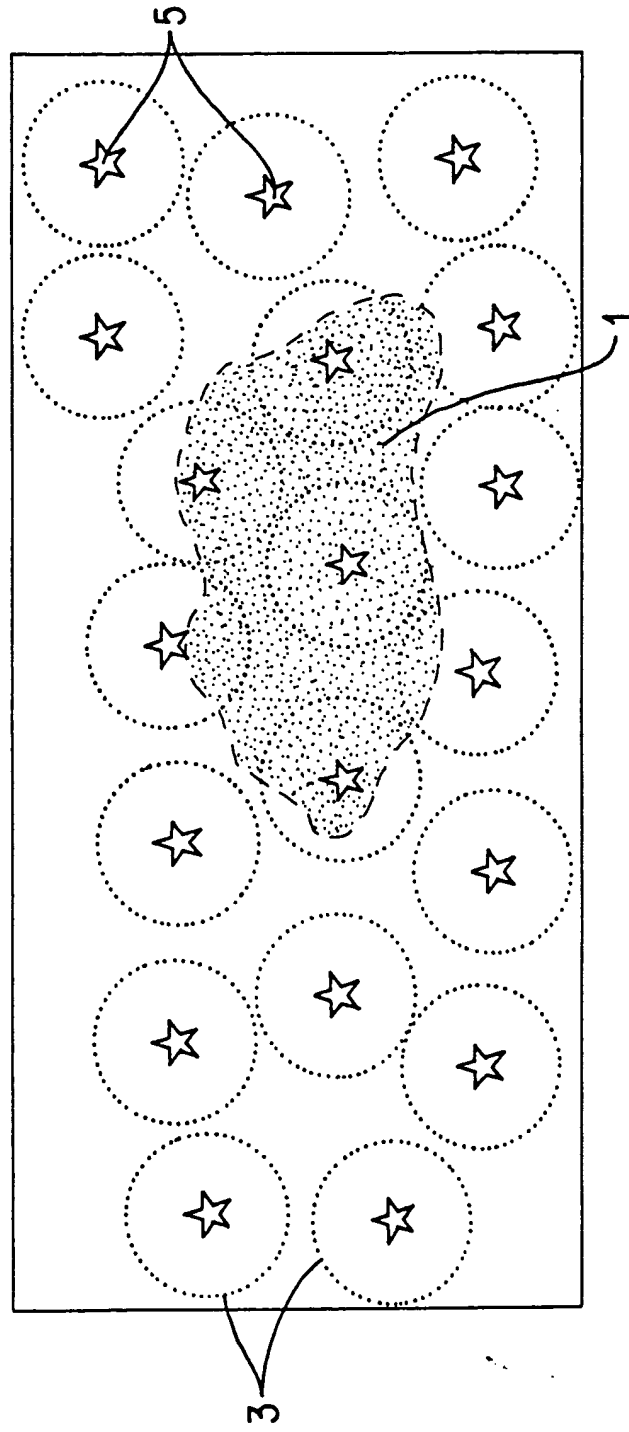


FIG. 1(b)

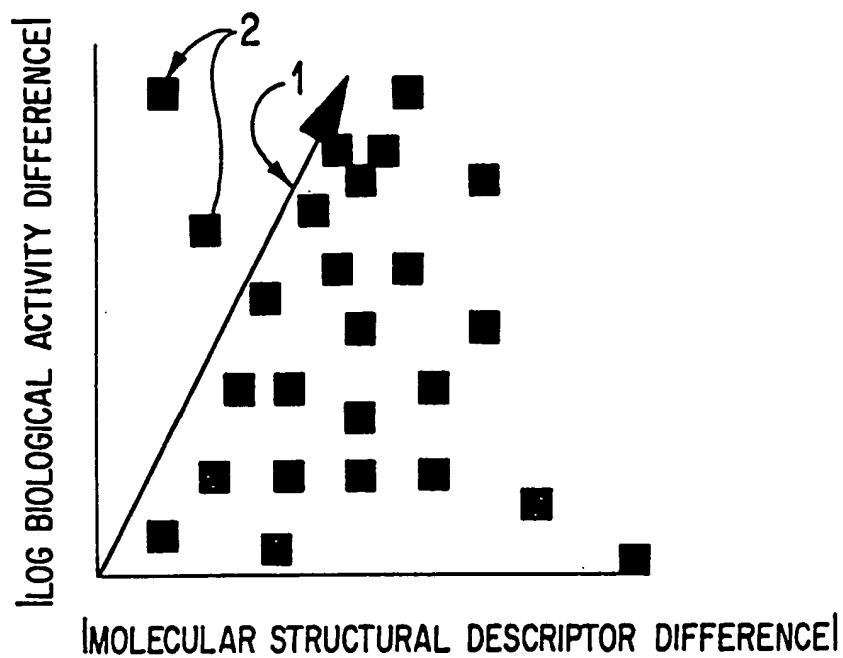


FIG. 2

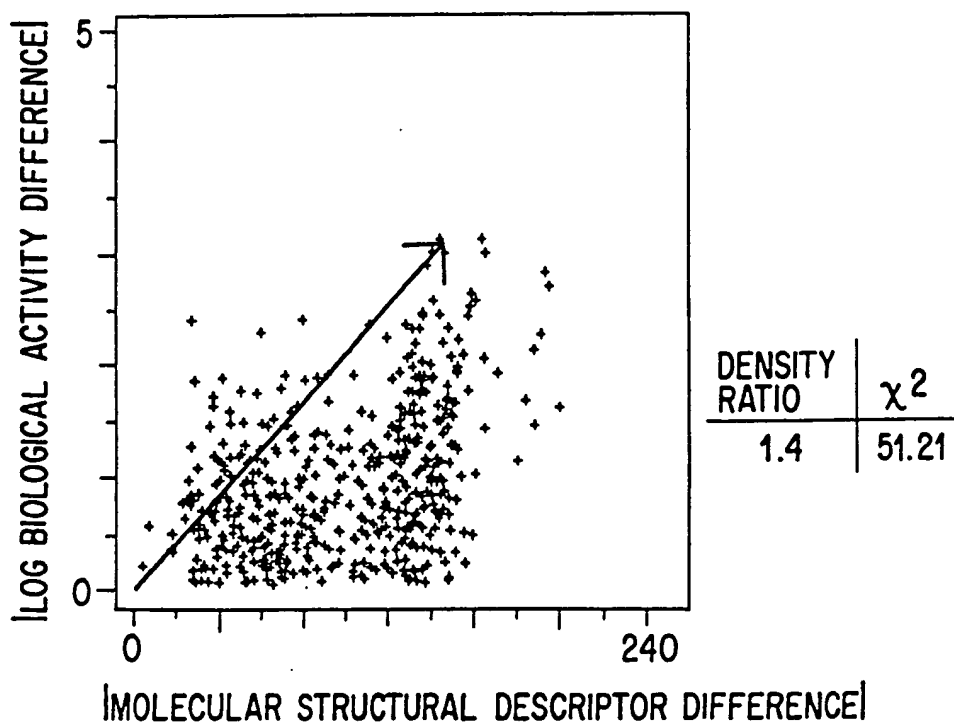


FIG. 3

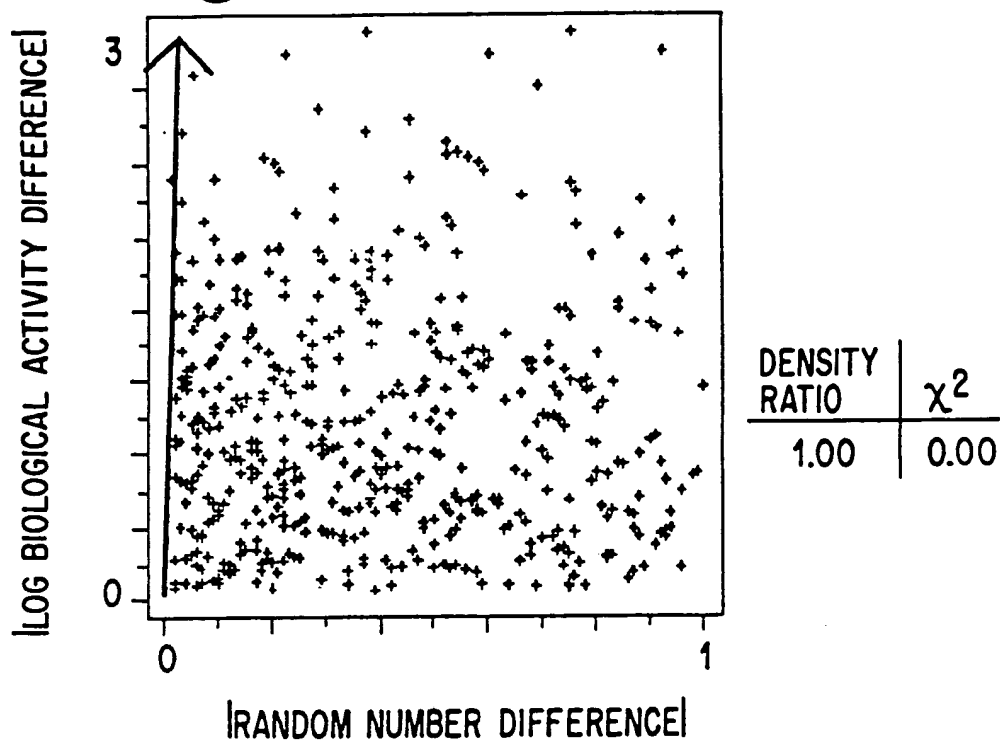


FIG. 4

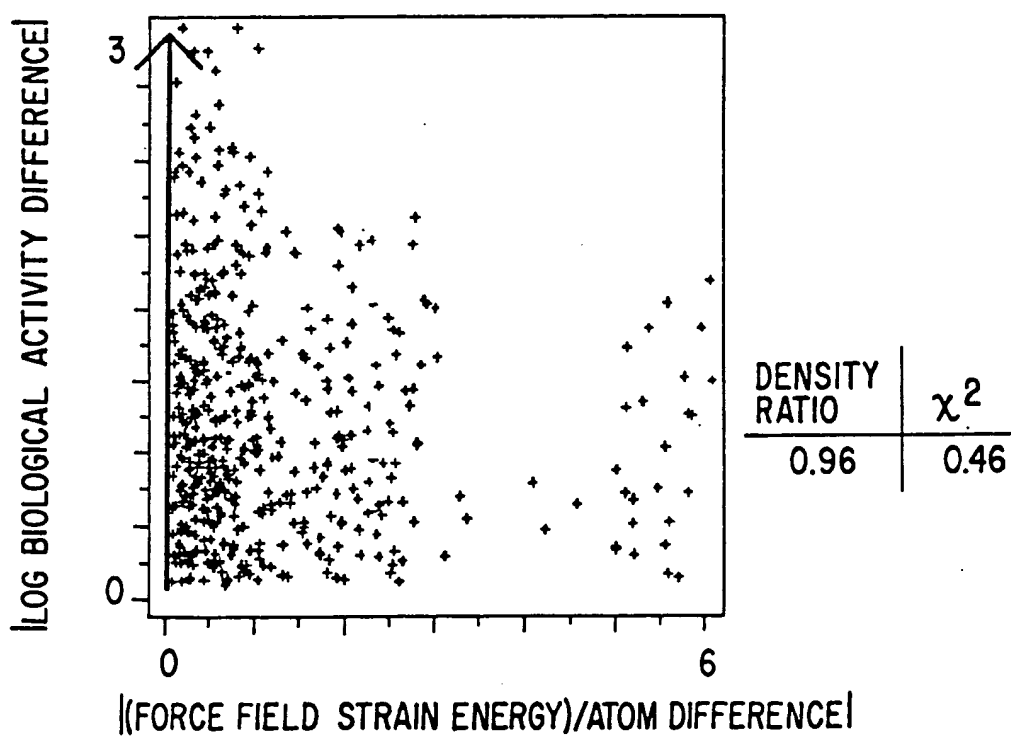
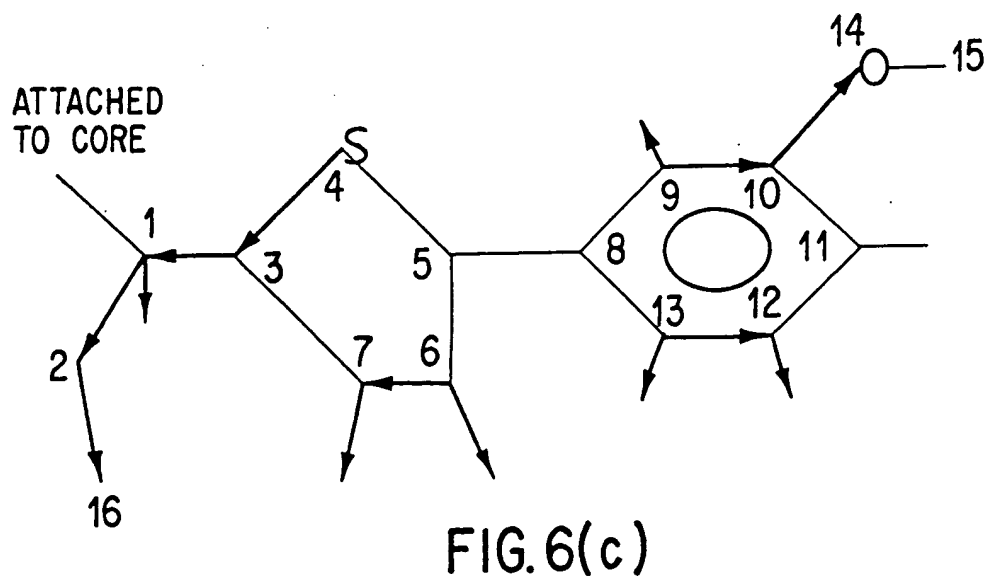
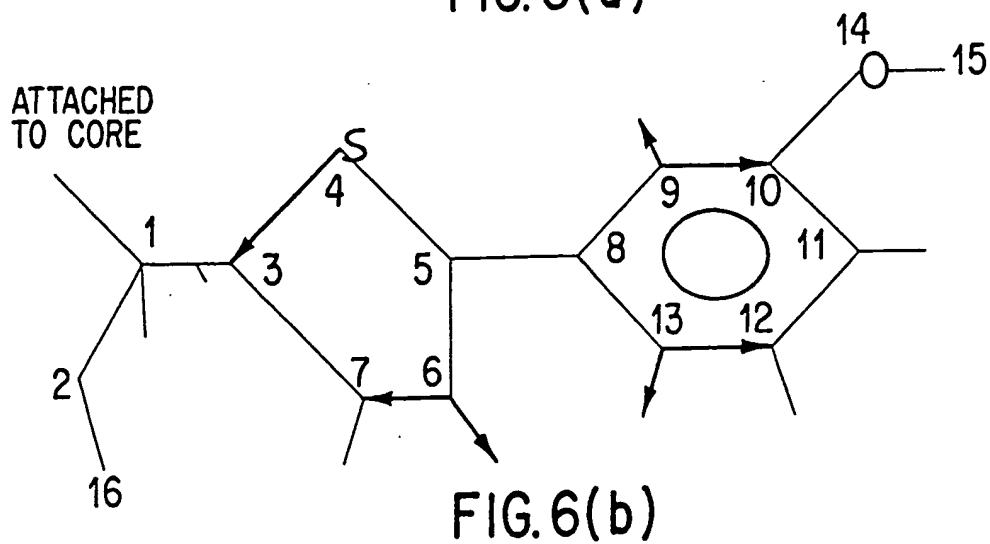
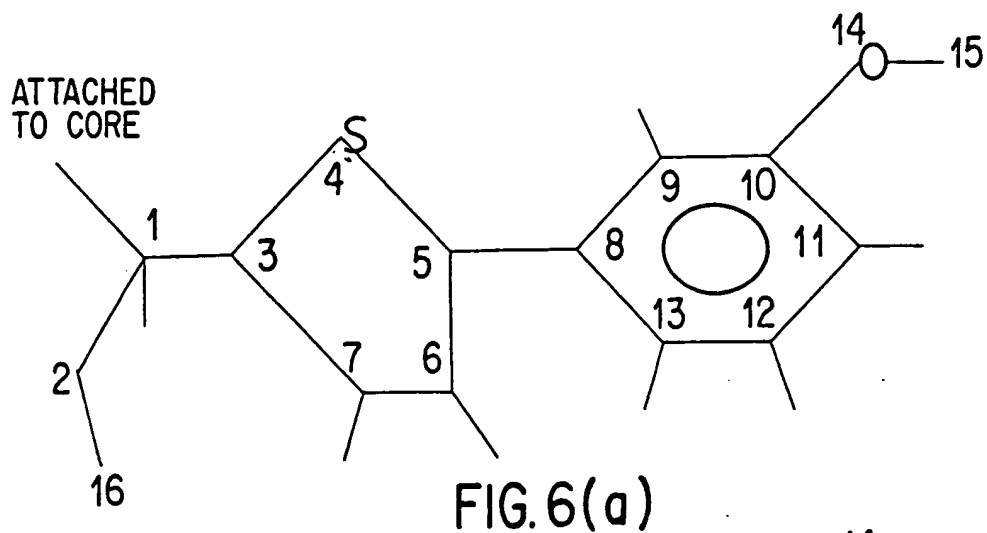


FIG. 5



DATA SET 2

Y-axis: LOG BIOLOGICAL ACTIVITY DIFFERENCE (0 to 5)

X-axis: |TOPO. COMFA DESCRIPTOR DIFFERENCE| (0 to 240)

FIG. 7(b)

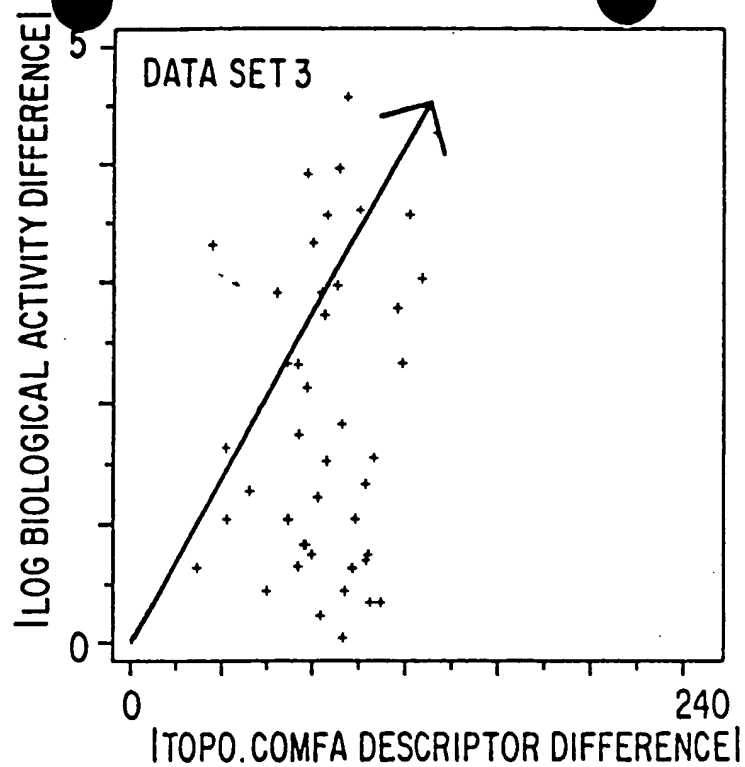


FIG.7(c)

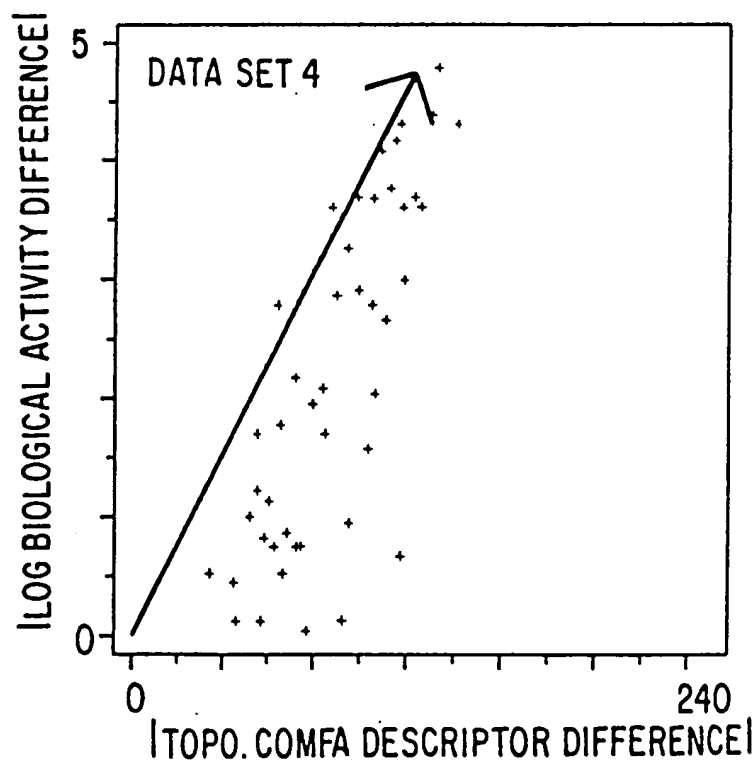


FIG.7(d)

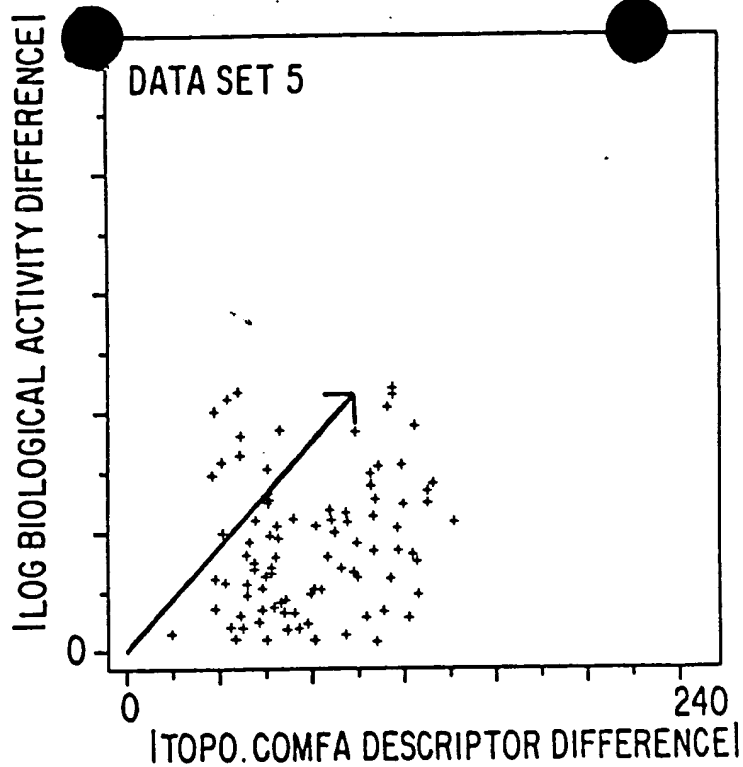


FIG.7(e)

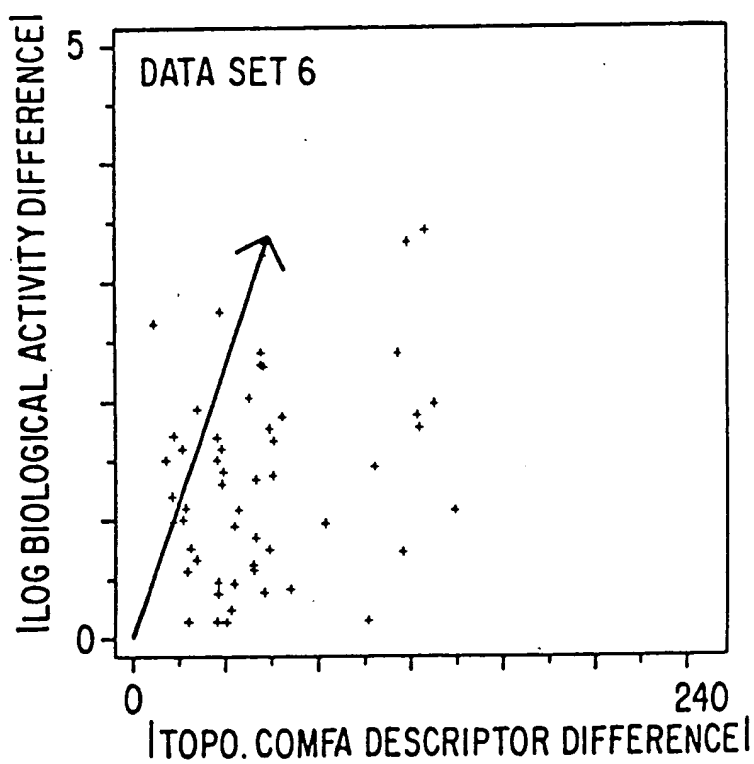


FIG.7(f)

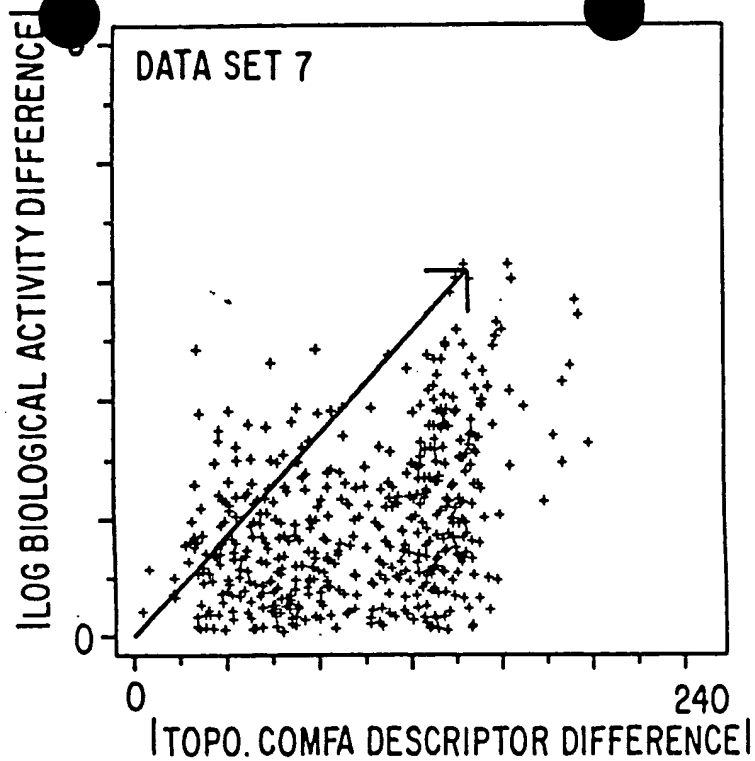


FIG.7(g)

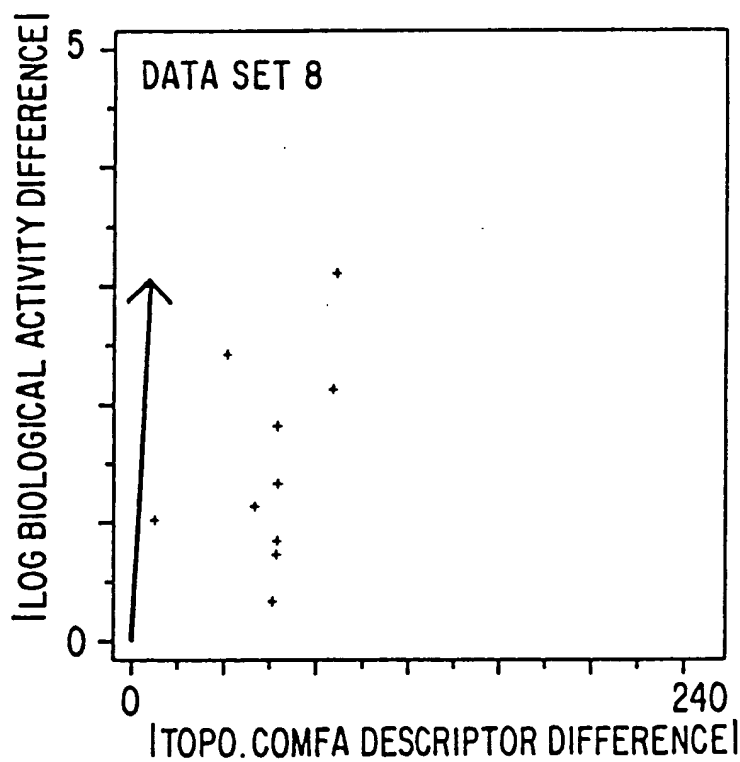


FIG.7(h)

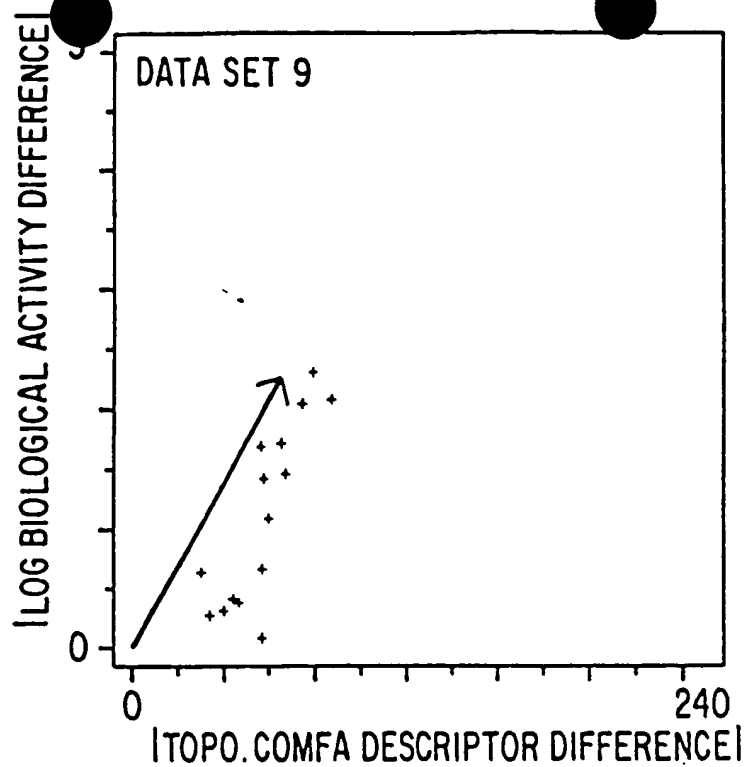


FIG.7(i)

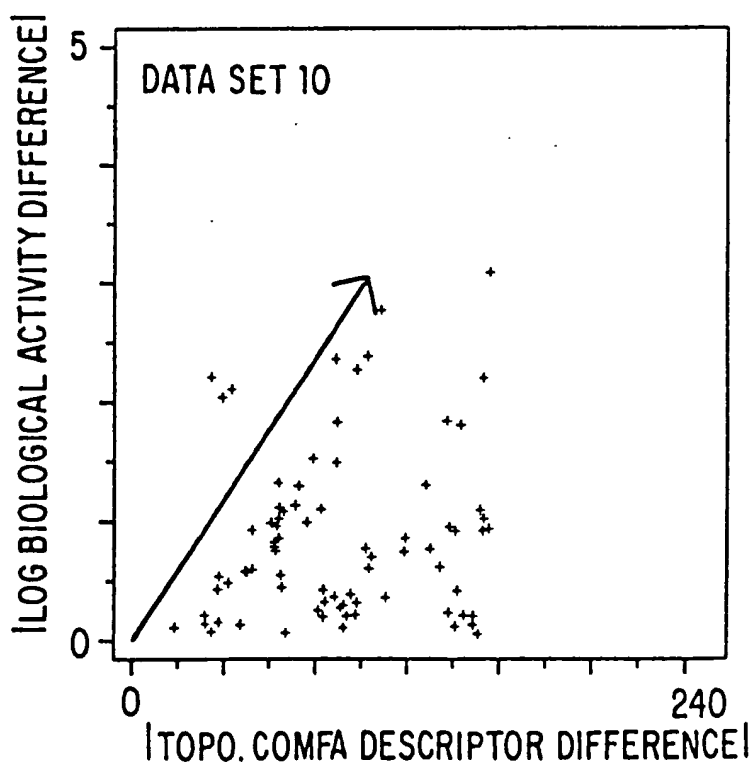


FIG.7(j)

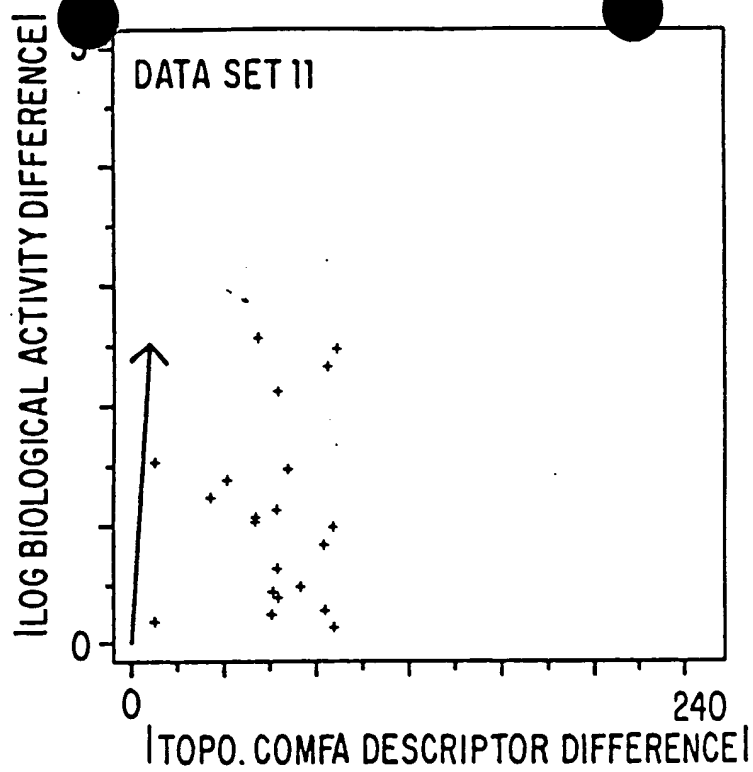


FIG.7(k)

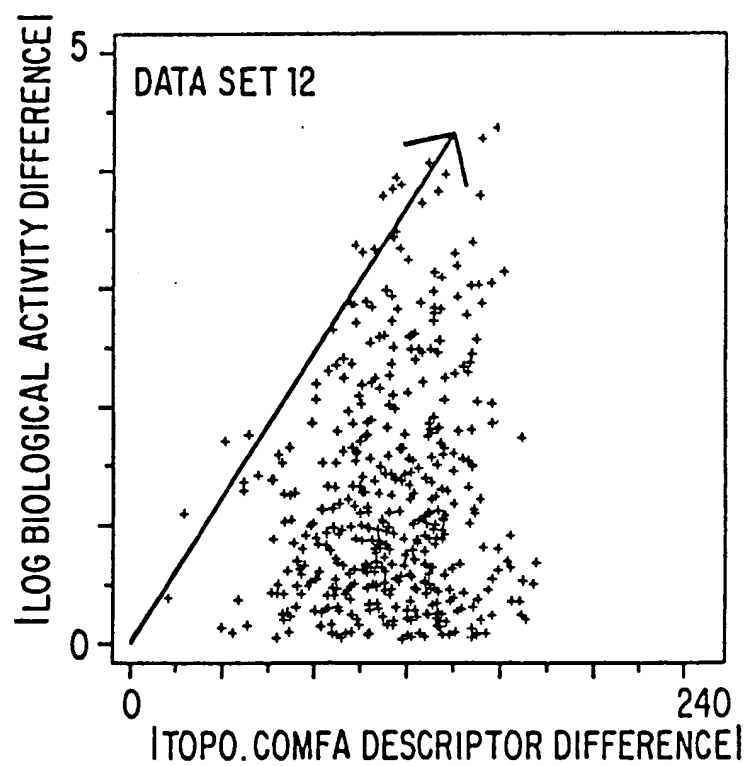


FIG.7(l)

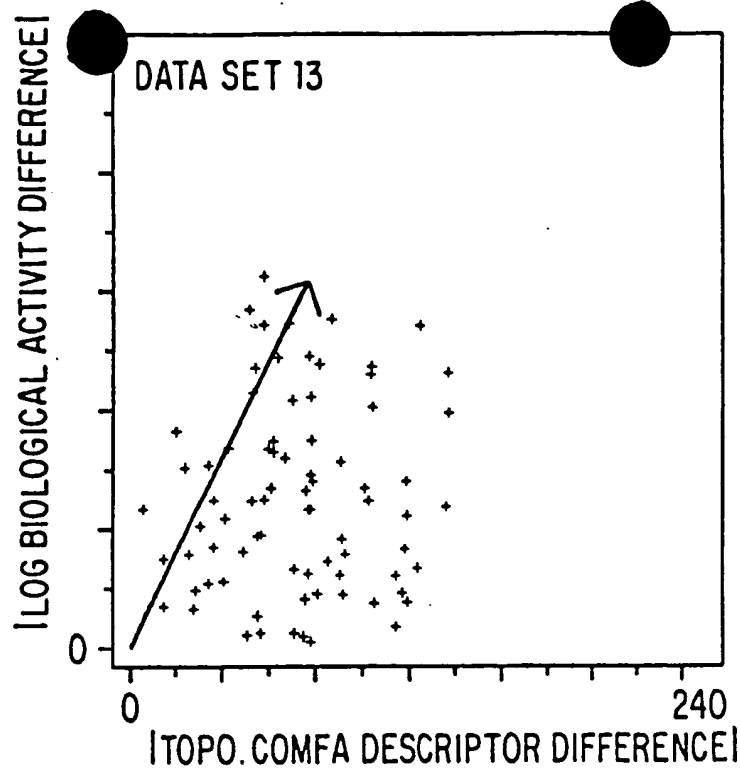


FIG.7(m)

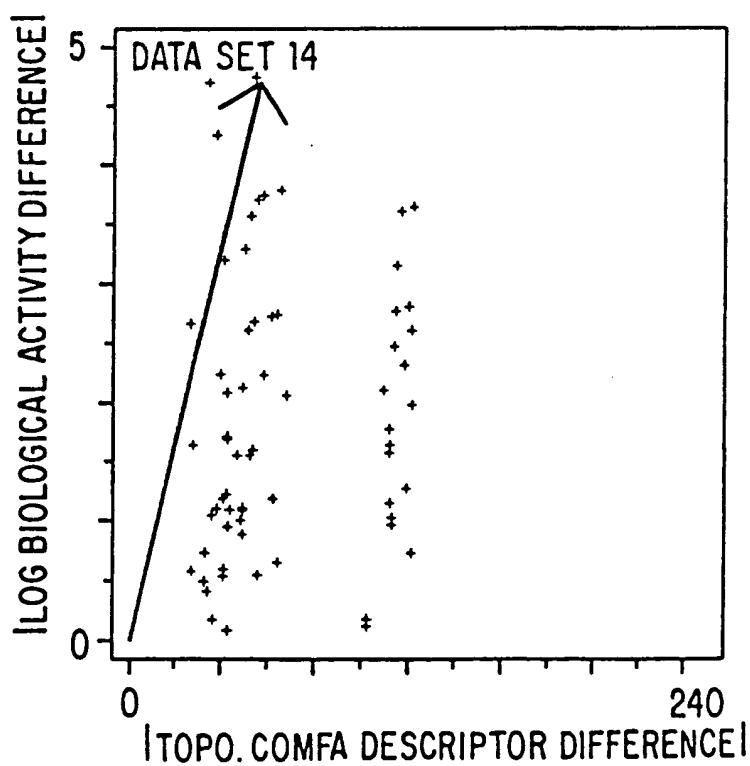


FIG.7(n)

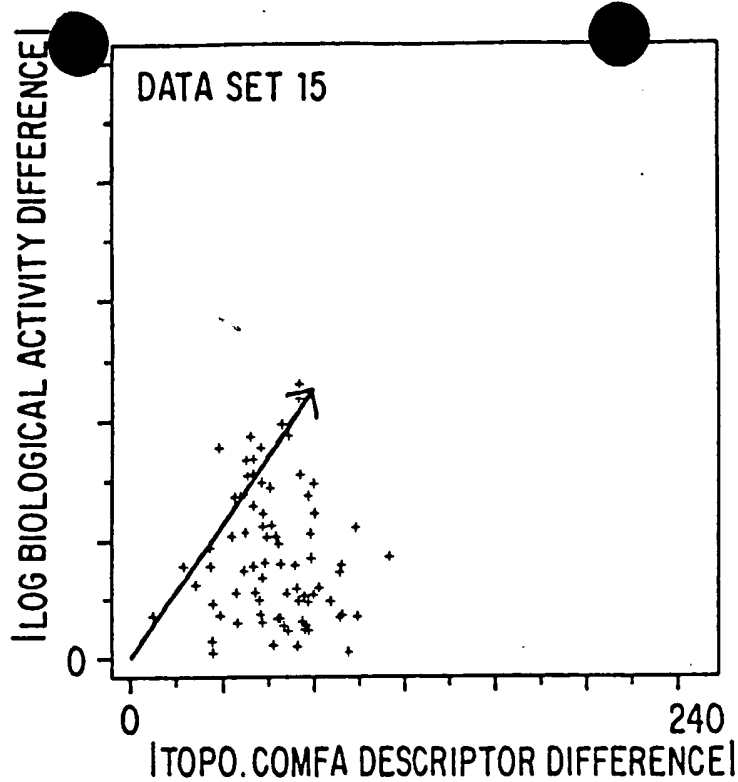


FIG.7(o)

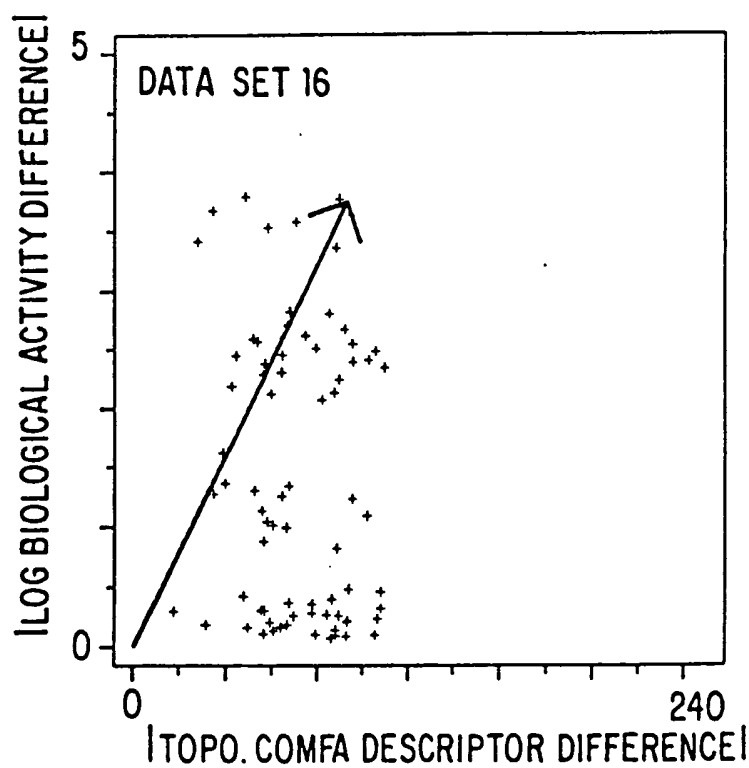


FIG.7(p)

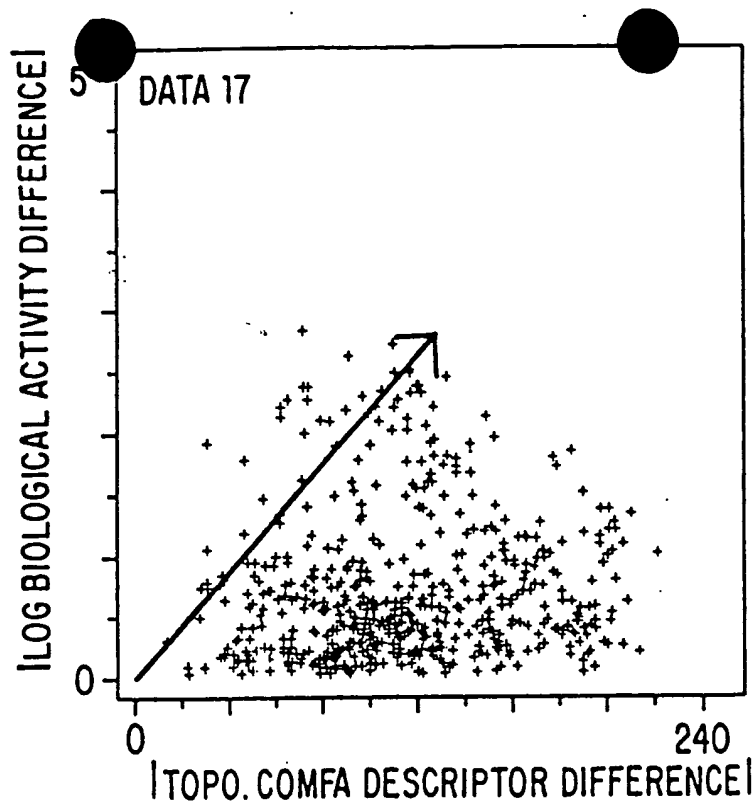


FIG.7(q)

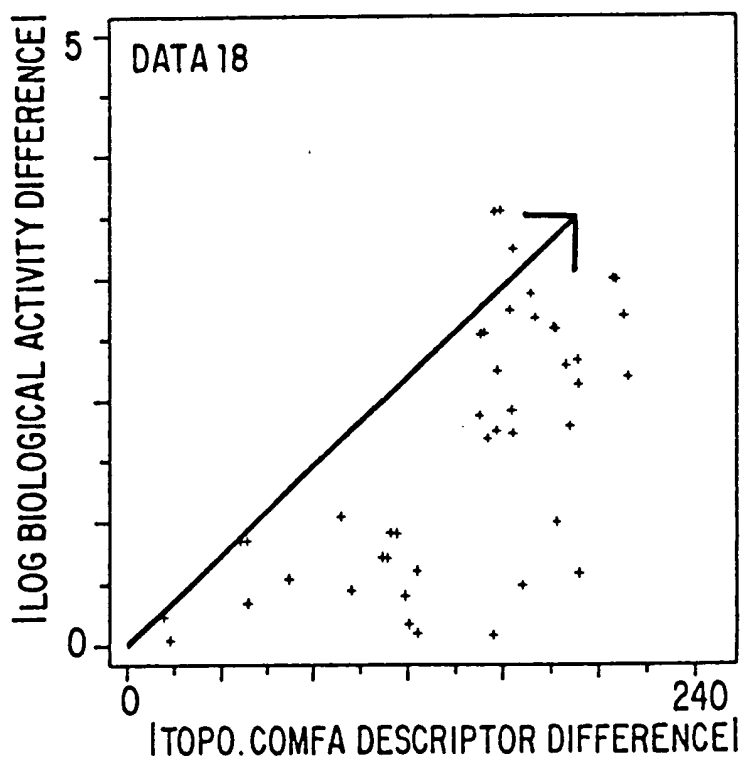


FIG.7(r)

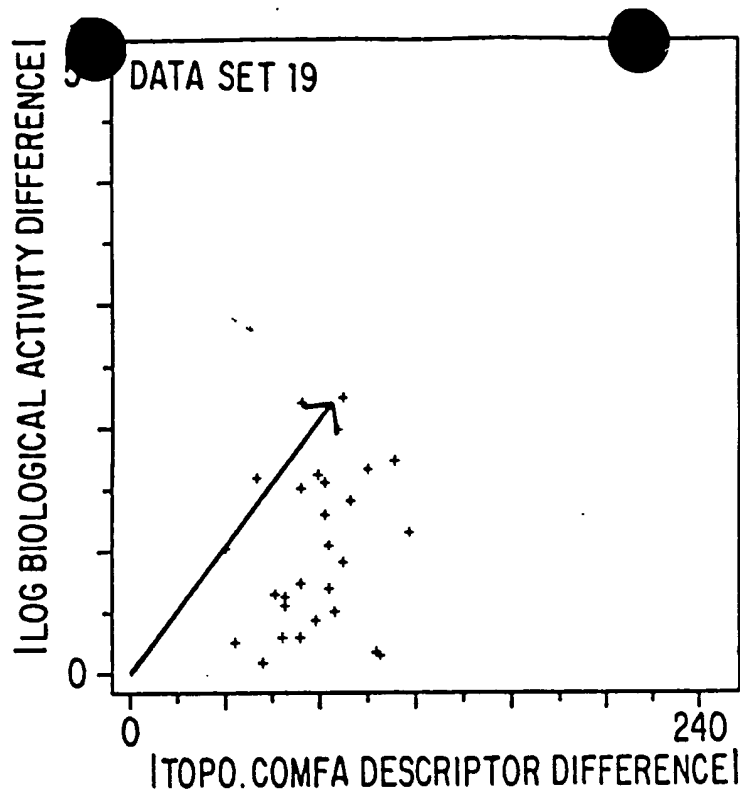


FIG.7(s)

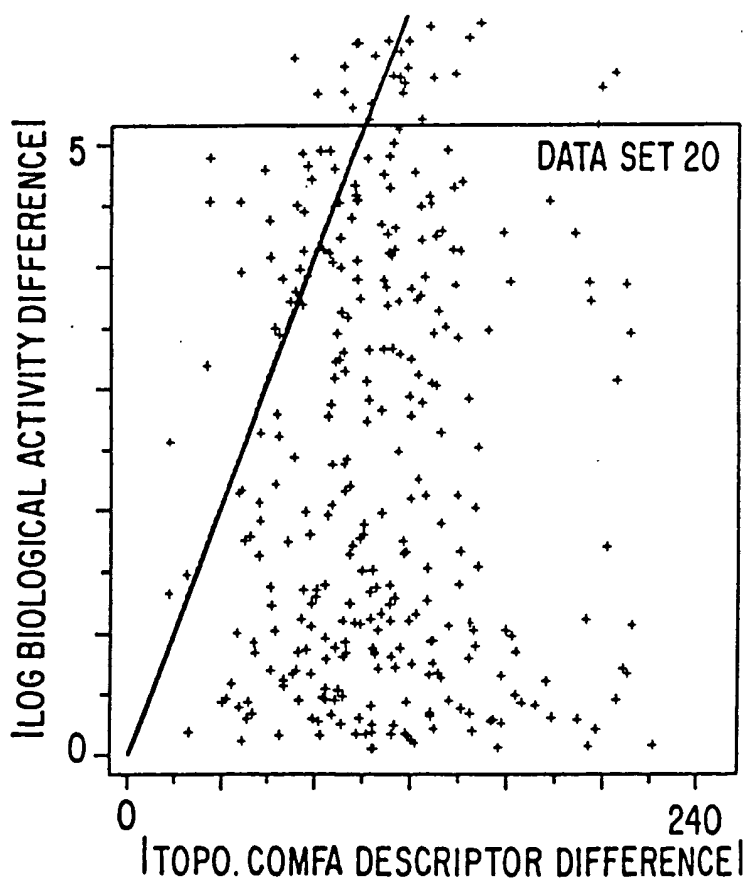


FIG.7(t)

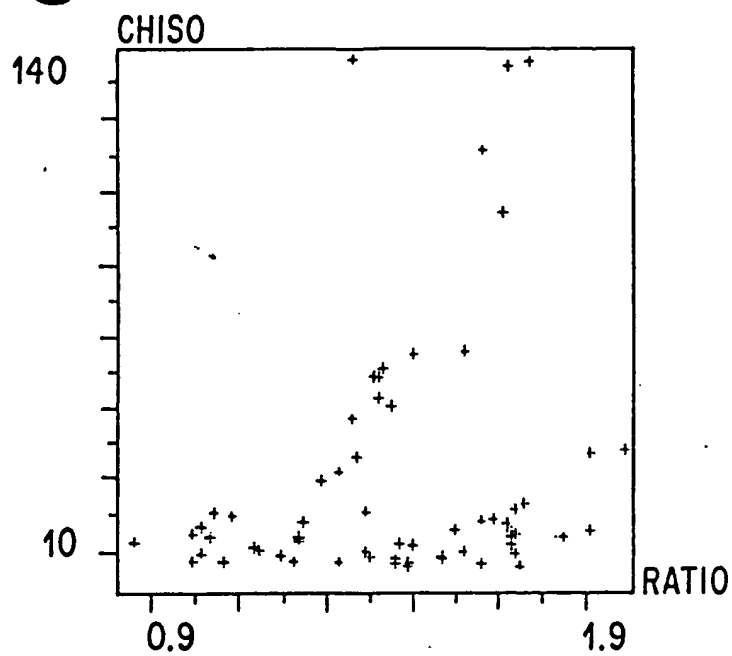


FIG. 8(a)

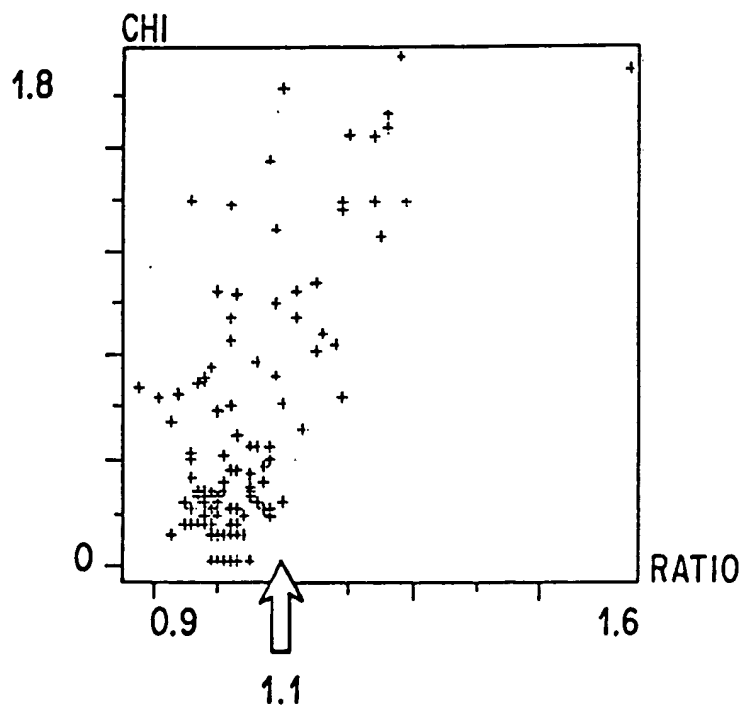


FIG. 8(b)

FF29260

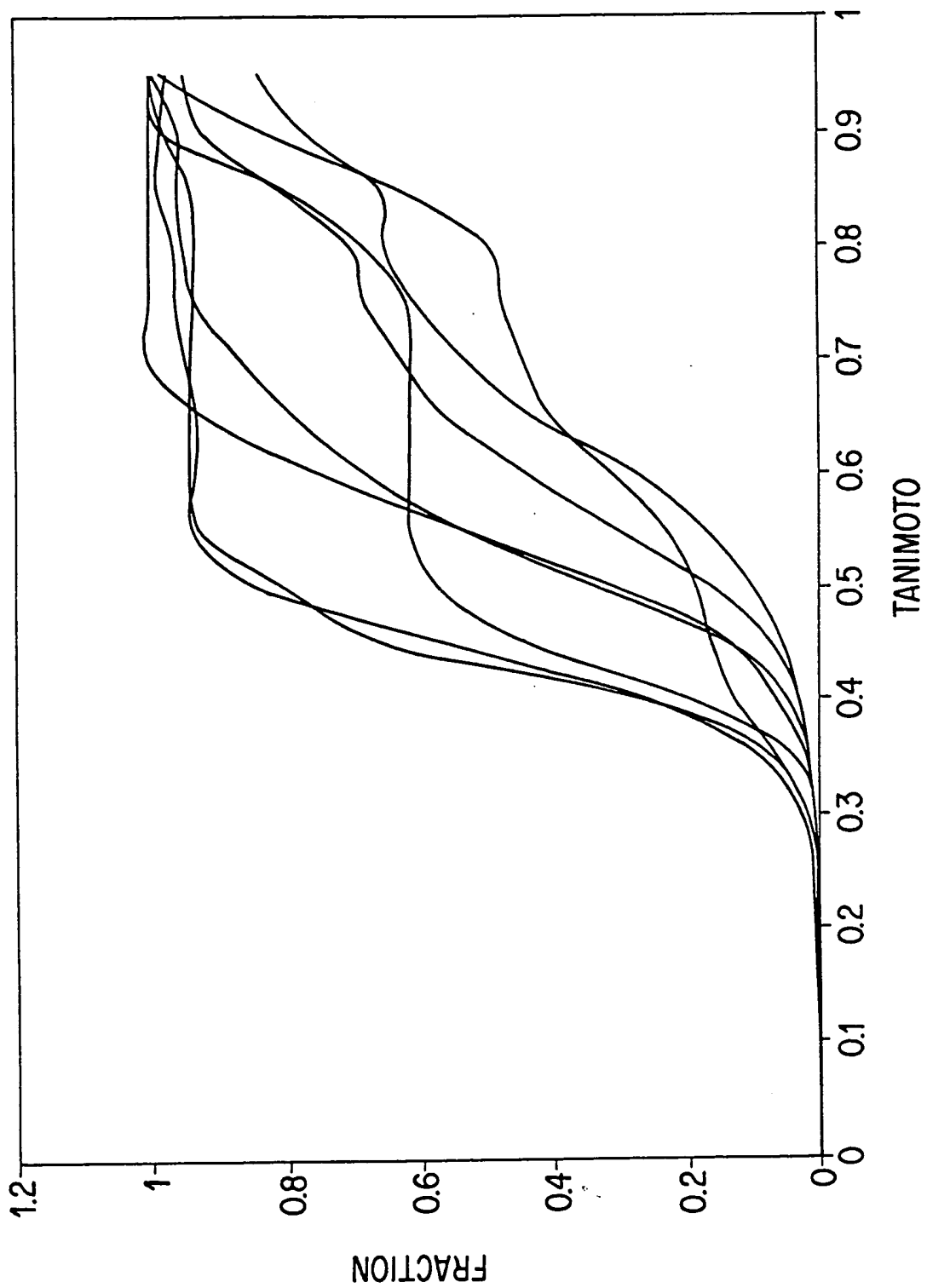


FIG. 9(a)

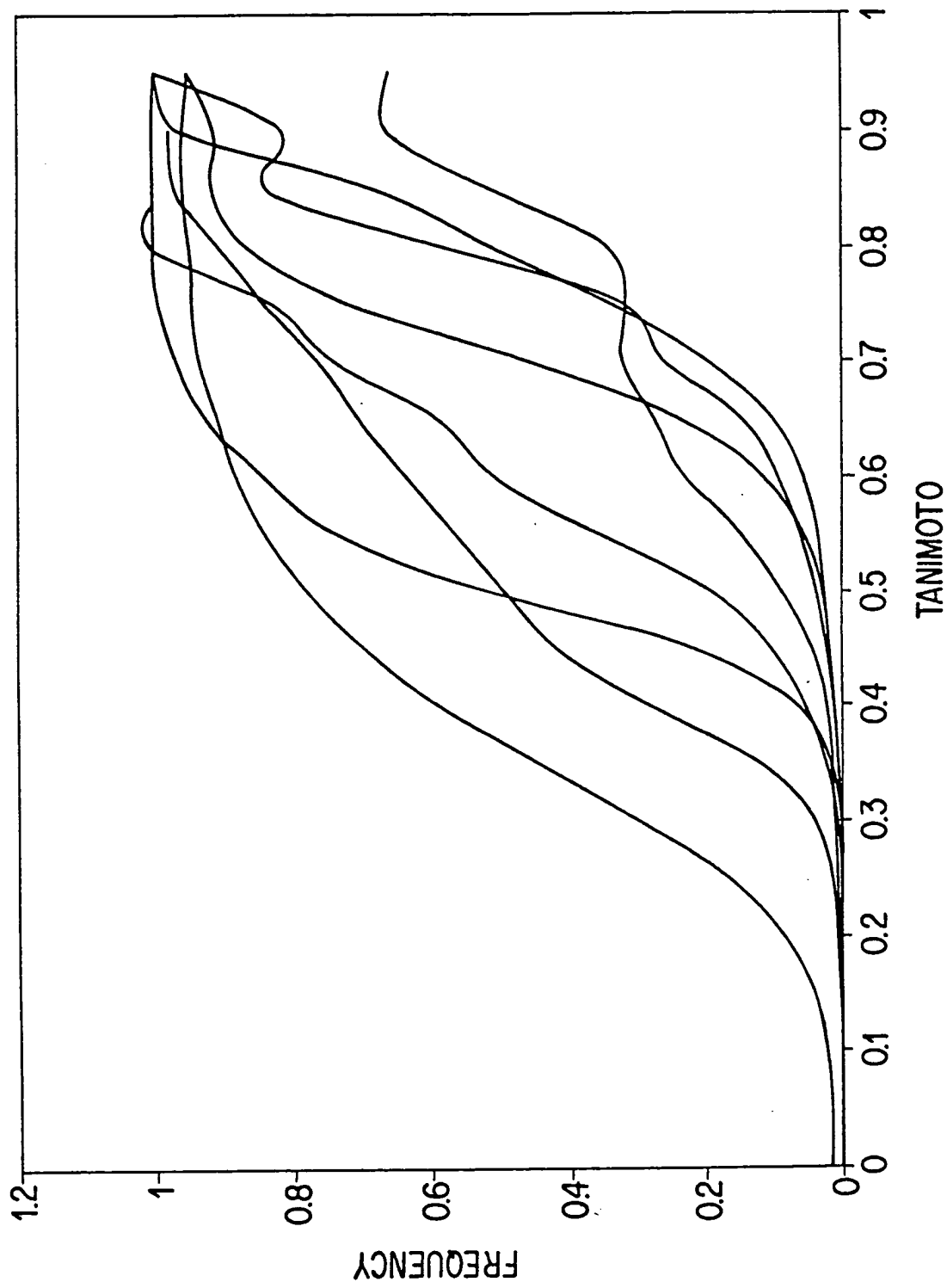
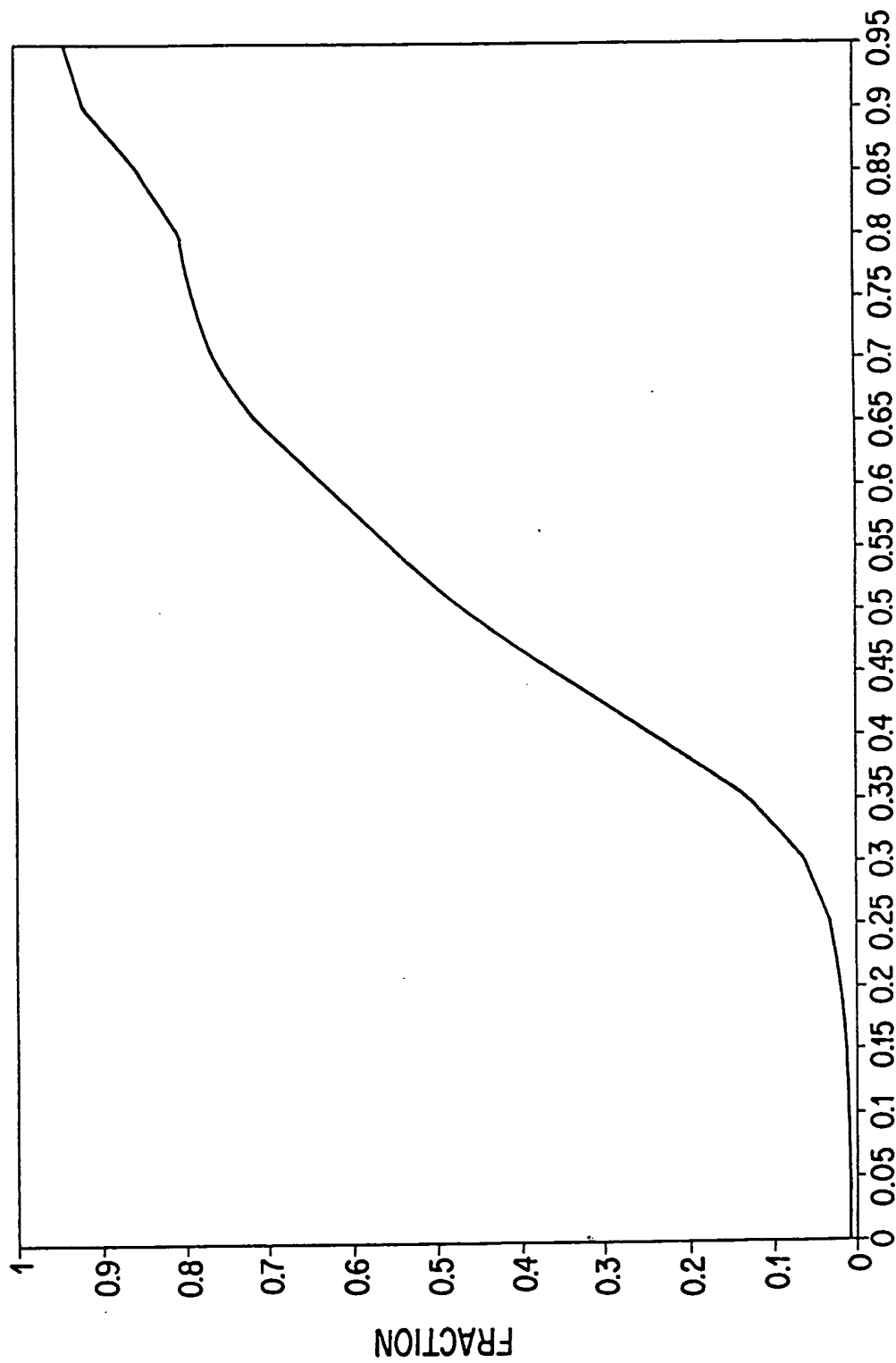


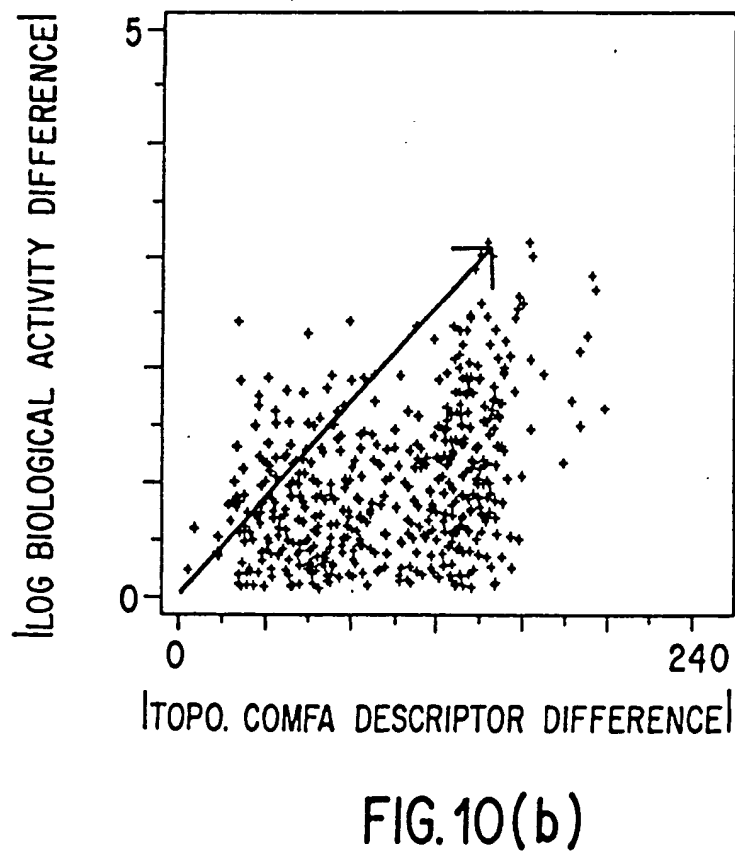
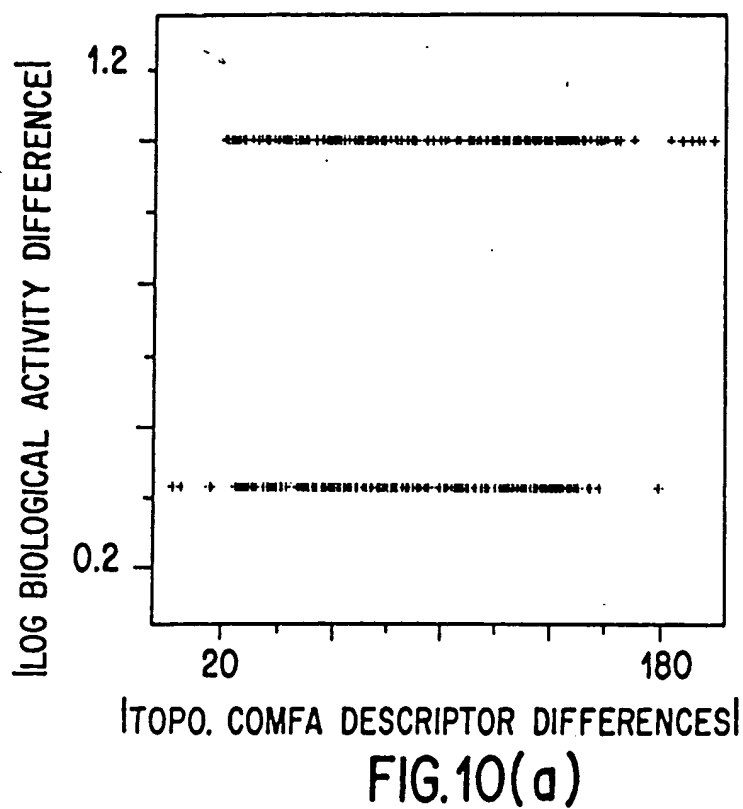
FIG. 9(b)

T09020" T294.60



TANIMOTO

FIG.9(c)



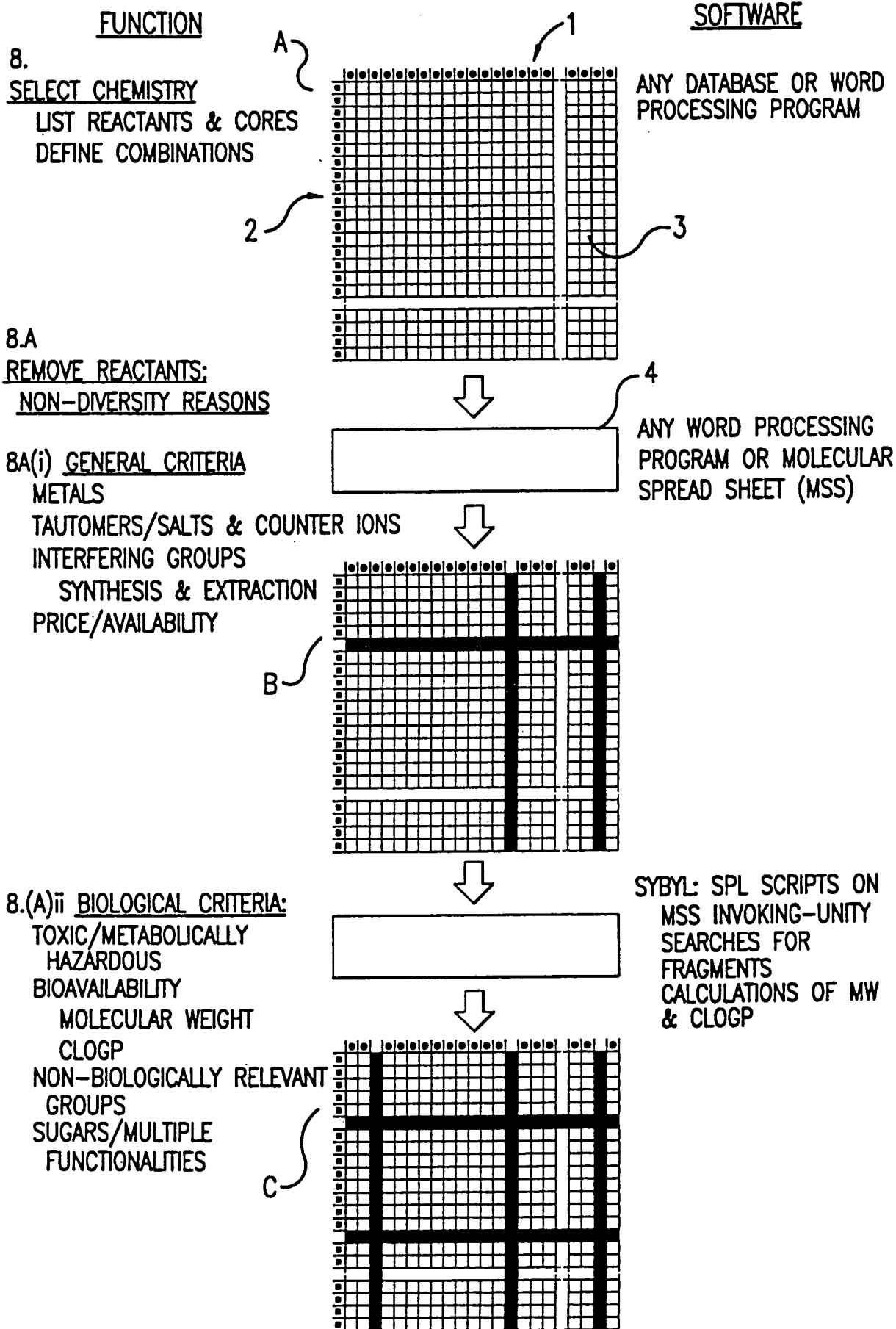


FIG.11(a)

8B

REMOVE NON-DIVERSE REACTANTS:

3D STRUCTURE GENERATION
TOPOMERIC CONFORMER
ALIGNMENT

CoMFA FIELD GENERATION:

HYDROGEN BOND FIELD
GENERATION

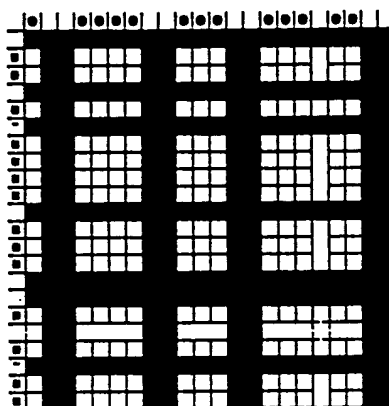
ROTATABLE BOND FIELD
ATTENUATION

CALCULATE FIELD
DIFFERENCES

CLUSTER

REACTANT SELECTION FROM
EACH CLUSTER

D



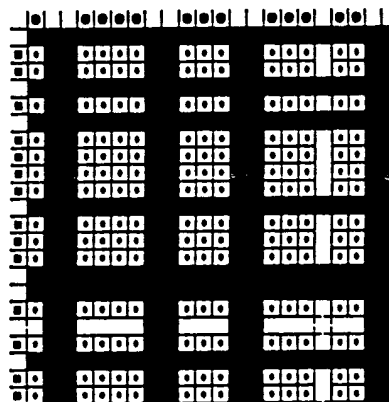
SYBYL: SELECTOR &
CONCORD 3.2.1
SPECIALIZED SOFTWARE:
APPENDIX "A"
(SYBYL: CoMFA
STERIC & MSS)

SYBYL: HIERCHICAL
CLUSTER - MSS
SYLBL: MSS

8C

COMBINE REACTANTS TO BUILD PRODUCTS

E



SYBYL: LEGION MSS

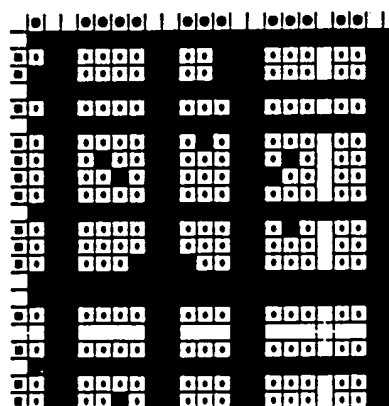
8D

REMOVE PRODUCTS:

NON-DIVERSITY REASONS

GENERAL CRITERIA:

F



SYBYL: SPL SCRIPTS
ON MSS

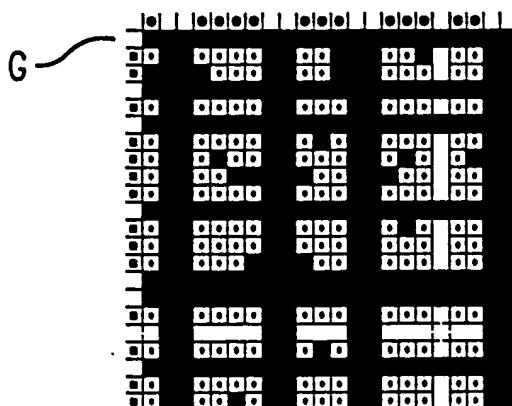


FIG.11(b)

0977674.0000
T05020.T09460

BIOLOGICAL CRITERIA:
METABOLICALLY HAZARDOUS
BIOAVAILABILITY
MOLECULAR WEIGHT
CLOGP

SYBYL: SPL SCRIPTS ON
MSS INVOKING -
UNITY SEARCHES FOR
FRAGMENTS
CALCULATIONS OF MW
& CLOGP



REMOVE NON-DIVERSE
PRODUCTS:

GENERATE TANIMOTO
2D FINGERPRINTS
SAMPLE PRODUCTS:
EXCLUDE TAN ≥ 0.85

UNITY

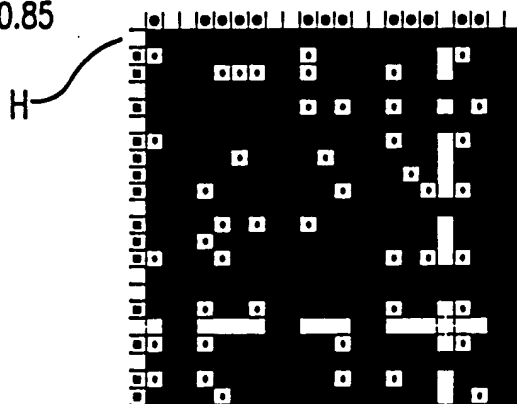
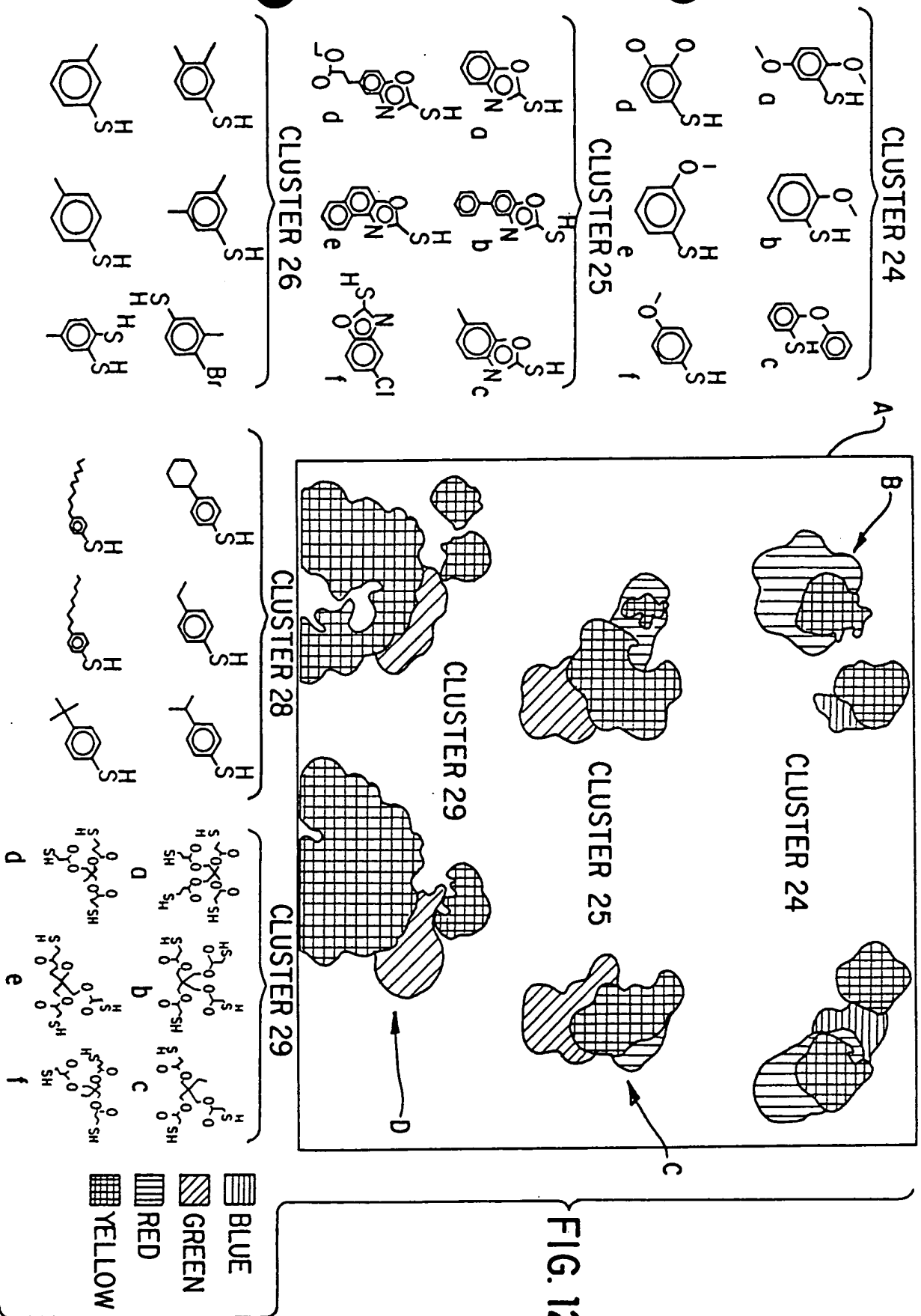


FIG. 11(c)



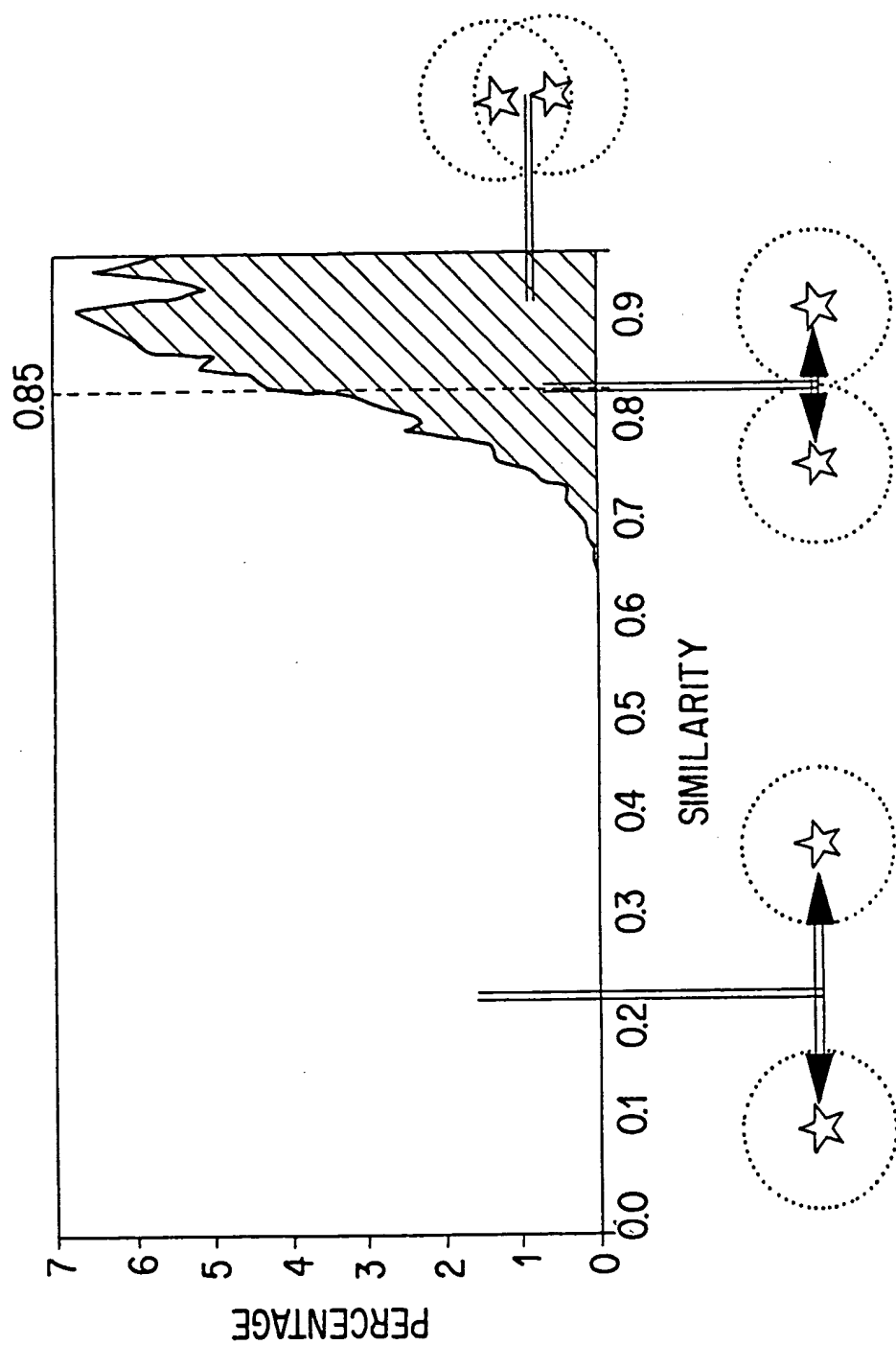


FIG.13

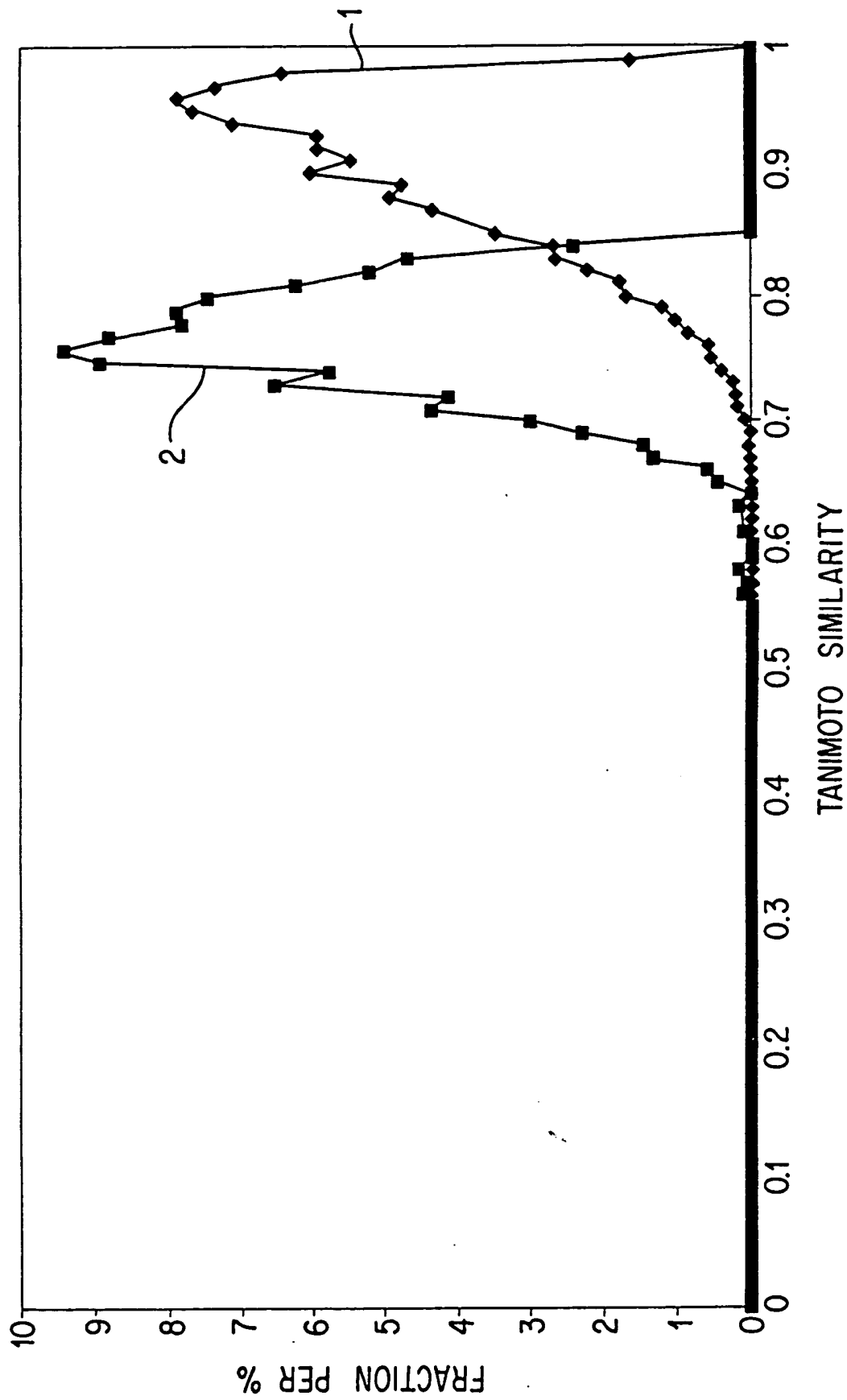


FIG. 14

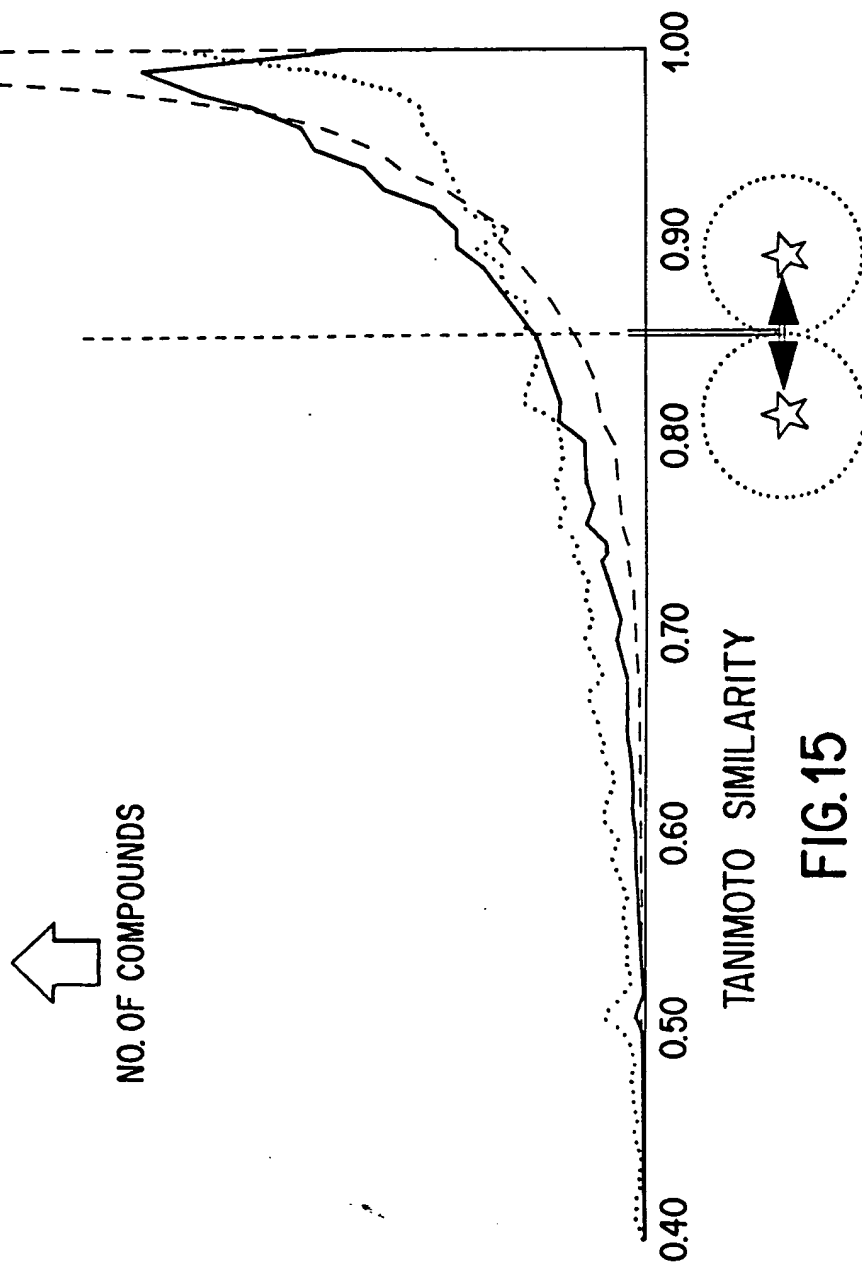


FIG.15